

Exploring beyond lithium-ion batteries with scattering techniques and advanced electrochemical analysis, spanning *ex situ* to real-time assessments

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Batteries are pivotal in driving the advancement of technologies that facilitate the transition to electromobility and renewable energy storage within grid systems. As new applications emerge, they introduce expanded demands such as increased energy density, rapid charging capabilities, a broad operational temperature range, and sustainability in both raw materials and manufacturing processes¹.

A global endeavour is in progress to meet these challenges by optimizing and enhancing the capabilities of next-generation technologies, such as lithium-sulfur batteries (LSBs)² or sodium-ion batteries (SIBs)^{3–5}. A shared characteristic among these advancements lies in the customizable carbonaceous electrodes (CCEs). The energy storage capacity of LSB cathodes and SIB anodes heavily depends on the morphology of CCEs sourced from various origins, spanning nanometer to angstrom length scales.⁶ For instance, the precipitation process in LSB still lacks complete comprehension, while the sodium storage mechanism in hard carbons presents uncertainties, prompting thorough investigations into the structure of non-graphitized carbons. Advanced characterization methods are pivotal in facilitating the essential progressions in battery technology⁷. Understanding the performance of novel materials, the intricacies of emerging chemical reactions, and diverse processes necessitates comprehensive characterization spanning from atomic-scale analysis to cell-level examinations.^{2–6} The swift advancements in synchrotron X-ray and neutron technologies open up fresh avenues for tackling these obstacles⁷. This 8th Baltic Electrochemistry Conference: Finding New Inspiration 2 contribution delves into recent advancements in comprehending the mechanisms at play in customizable carbonaceous anodes and cathodes. It emphasizes employing scattering techniques, spanning from *ex situ* to real-time assessments, along with state-of-the-art electrochemical analysis and experiments conducted at large-scale facilities.

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References

1. S. Bobba, S. Carrara, J. Huisman, F. Mathieux and C. Pavel, *Critical Raw Materials for Strategic Technologies and Sectors in the EU - a Foresight Study*, 2020.
2. L. Kalder, A. Olgo, J. Lührs, R. Härmas, J. Aruväli, P. Partovi-Azar, A. Petzold, E. Lust, E. Härk, Interlayer Spacing of Hard Carbon as a Quantified Structural Parameter for Sodium-Ion Batteries. Combined Analysis by WAXS and SANS, *Energy Storage Materials*, 2024, under revision.
3. A. Adamson, R. Väli, M. Paalo, J. Aruväli, M. Koppel, R. Palm, E. Hark, J. Nerut, T. Romann, E. Lust, A. Jänes, *RSC Adv.*, 2020, **10**, 20145–20154.
4. K. Schutjajew, P. Giusto, E. Härk and M. Oschatz, *Carbon N. Y.*, 2021, **185**, 697–708.
5. S. Risse, E. Härk, B. Kent, M. Ballauff, *ACS Nano*, 2021, **13(9)**, 10233–10241.
6. E. Härk, A. Petzold, G. Goerigk, S. Risse, I. Tallo, R. Härmas, E. Lust and M. Ballauff, *Carbon N. Y.*, 2019, **146**, 284–292.
7. E. K. J. Allan-Cole, I. Arçon, M. Bianchini, C. Didier, R. Dominko, M. Fehse, Z. Gao, M. Guizar-Sicairos, E. Härk, K. Hatzell, T. Jousseume, M. Kavčič, Z. Lu, F. Marini, J. Mata, V. K. Peterson, E. Principi, M. Sadd, A. Senyshyn, P. R. Shearing, S. Tardif, M. F. Toney, C. Villevieille, A. Vizintin, A. Iadecola, S. Lyonard, A. Matic, L. Stievano. Roadmap to operando analyses of batteries at large-scale facilities: 2. Small Angle Scattering (SAXS/USAXS/SANS/USANS)– *Journal of Physics: Energy*, 2024 - under revision.